

Guanidine, N,N''-(iminodi-8,1-octanediyl)bis-
13516-27-3 | DTXSID7042015

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 165 °C

Global applicability domain: Outside

Local applicability domain index: 1.97e-01

Confidence level: 5.32e-01

Nearest Neighbors from the Training Set

Image not found

Phenformin

Measured: 177

Predicted: 169

Image not found

Chlorguanide

Measured: 129

Predicted: 136

Image not found

1-(o-Tolyl)biguanide

Measured: 144

Predicted: 150

Image not found

Amiloride

Measured: 241

Predicted: 174

Image not found

Imidodicarbonimidic diamide

Measured: 136

Predicted: 139